Title: Magnetic circular dichroism and aromatic compounds

Author: Petr Štěpánek


Abstract: The thesis presents a series of studies concerning magnetic circular dichroism (MCD), a spectroscopic method, which experienced an intense theoretical development in the recent years. New computational codes opened possibilities to calculate MCD spectra of larger and more varied molecules than was possible in the past. In the presented studies, we took the advantage of the new computational codes to broaden the possible span of applications of the MCD technique. As an example, we present MCD as a method useful for obtaining information about the structure of fullerenes. We also studied the influence of the molecular conformation and the explicit and implicit solvent models on the MCD spectra of aromatic amino acids using the newly implemented alternative computational protocol based on sum-over-states calculations. We have also theoretically predicted spectra of the nuclear spin circular dichroism (NSCD), a potential new high-resolution spectroscopy.

Keywords: magnetic circular dichroism, quantum-chemical calculations, density functional theory, nuclear spin circular dichroism